SET B

M.SC. CHEMISTRY
SECOND SEMESTER
QUANTUM CHEMISTRY-II
MSC – 204

[USE OMR FOR OBJECTIVE PART]

Duration: 1:30 hrs. **Full Marks: 35**

(Objective)

Time: 15mins. **Marks: 10**

Choose the correct answer from the following: ***1×10=10***

1. Which theorem provides a framework for obtaining approximate solutions to the Schrödinger equation by optimizing a trial wavefunction?
   a. Heisenberg Uncertainty Principle
   b. Variation theorem
   c. Perturbation theorem
   d. Pauli's exclusion principle

2. What does the perturbation theorem provide a systematic method for?
   a. Finding exact solutions to the Schrödinger equation
   b. Solving systems with time-dependent Hamiltonians
   c. Calculating corrections to energy levels of a known system
   d. Describing the behavior of particles in strong magnetic fields

3. According to Huckel theory, what type of orbitals participates in the molecular orbital formation?
   a. Atomic orbitals from all atoms in the molecule
   b. Only s orbitals from all atoms in the molecule
   c. Only p orbitals from all atoms in the molecule
   d. Only d orbitals from all atoms in the molecule

4. In the context of quantum mechanics, what does the term "anti-symmetry" refer to?
   a. The symmetry of wavefunctions under rotation
   b. The symmetric behavior of particles in a magnetic field
   c. The exchange behavior of identical particles
   d. The behavior of particles under the action of a potential energy field

5. Number of radial nodes in 3d orbital is -
   a. 4
   b. 0
   c. 2
   d. None of the above

6. The value of [x,x] is (where x=position operator)
   a. 0
   b. 6
   c. 5
   d. None of the above

7. For 1s orbital, the radial distribution plot is -
   a. Decayed
   b. Ex
   c. Depends upon molecule
   d. None of the above

8. Slater Determinant involves orbital part along with -
   a. Spin part
   b. Momentum part
   c. Energy part
   d. None of the above

9. What does the Born-Oppenheimer approximation primarily aim to simplify?
   a. Electron-electron interactions
   b. Electron-nucleus interactions
   c. Nuclear-nuclear interactions
   d. Electron-spin interactions

10. Hamilltonian operator is also known as -
   a. Total energy operator
   b. Kinetic energy operator
   c. Potential energy operator
   d. Position operator

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Descriptive

Time : 1 hr. 15 mins. **Marks : 25**

[Answer question no.1 & any two (2) from the rest]

1. a. Show that position and momentum doesn't commute on the same Axis. **3+2=5**

   b. Explain the perturbation theorem and its role in quantum mechanics

2. a. How linear momentum is related with kinetic energy? Show mathematically. **2+2+2+4 =10**

   b. Find out the angular momentum operator in y-axis using the cross product operation.

   c. Draw the radial distribution curve for 3p and 3d orbitals.

   d. The unperturbed energy levels of a system are $E_0=0$, $E_1=2$, $E_2=4$. The 2^{nd} order correction to energy for 2^{nd} excited state in presence of perturbation V for which $V_{10}=2$, $V_{20}=4$, $V_{12}=6$ has found to be?

3. a. Find out the value of 'n' and 'l' from the given expression $R=(1-r)e^{-r/3a0}$ **2+3+5 =10**

   b. Draw the angular node for 2p and 3d orbital. What is the number of radial node for 4f orbital?

   c. Calculate (i) Excitation energy (ii) Total energy (iii) Π-bond formation energy (iv) Delocalization energy of Cyclobutadiene using Huckel Molecular Orbital theory?

4. a. If the right half of the 1-D box is perturbed by a potential 'V'; Calculate the 1^{st} order correction in ground state energy. **3+2+2+2 +1=10**

   b. Write the volume element for H-atom considering both radial and angular part.

c. What is the average value of radius vector for 2s orbital for H-atom?

d. Define a many-electron wave function and explain its components.

e. Explain whatBorn-Oppenheimer approximation is.

5. a. Using Variation theorem, find the energy for a particle in a 1-D box having the wave function $\Psi = \text{Sin}\ (\frac{n\Pi x}{l})$and find if the wavefunction is acceptable or not? **5+3+2 =10**

b. What is Laplacian operator? How this operator is involved in total energy operator?

c. Find the commutation value for $[x, \sin(p_x)]$

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